

# REPORT DOCUMENTATION PAGE

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MEMORANDUM FOR PRS (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)

08 February 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-028**

Christe, K.O. (ERC), Zhang, X. (USC), Sheehy, J. (PRSP), Bau, R. (USC), "The tetrafluorohalogen cations  $\text{ClF}_4$ ,  $\text{SeF}_4$ , and  $\text{TeF}_4$ "

**American Chemical Society Mtg (San Francisco, CA, 26-30 Mar 2000)**  
**(Deadline: 10 Mar 2000)**

**(Statement A)**

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.

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3. This request has been reviewed by the STINFO for: a.) changes if approved as amended, b.) appropriateness of distribution statement, c.) military/national critical technology, d.) economic sensitivity, e.) parallel review completed if required, and f.) format and completion of meeting clearance form if required

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4. This request has been reviewed by PRS for: a.) technical accuracy, b.) appropriateness for audience, c.) appropriateness of distribution statement, d.) technical sensitivity and economic sensitivity, e.) military/national critical technology, and f.) data rights and patentability

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APPROVED/APPROVED AS AMENDED/DISAPPROVED

\_\_\_\_\_  
PHILIP A. KESSEL Date  
Technical Advisor  
Propulsion Science and Advanced Concepts Division

## The tetrafluorohalogen cations $\text{ClF}_4^+$ , $\text{BrF}_4^+$ , and $\text{IF}_4^+$ and their isoelectronic counterparts $\text{SF}_4$ , $\text{SeF}_4$ , and $\text{TeF}_4$

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The crystal structure of the 1:1 adduct,  $\text{ClF}_5\text{SbF}_5$ , was determined and shown to contain discrete  $\text{ClF}_4^+$  and  $\text{SbF}_6^-$  ions. The  $\text{ClF}_4^+$  structure can be described as a trigonal bipyramid with two longer more ionic axial bonds and two shorter more covalent equatorial bonds. The third equatorial position is occupied by a sterically active free valence electron pair on chlorine. The coordination about the chlorine atom is completed by two longer fluorine contacts in the equatorial plane resulting in the formation of infinite zigzag chains of alternating  $\text{ClF}_4^+$  and -fluorine bridged  $\text{SbF}_6^-$  ions. Electronic structure calculations were carried out for the isoelectronic series  $\text{ClF}_4^+$ ,  $\text{BrF}_4^+$ ,  $\text{IF}_4^+$  and  $\text{SF}_4$ ,  $\text{SeF}_4$ ,  $\text{TeF}_4$ , and their vibrational spectra and force fields were revised. A simple method was developed for modeling the effects of fluorine bridging on the individual  $\text{ClF}_4^+$  and  $\text{SbF}_6^-$  ions in the infinite  $-(\text{ClF}_4^+-\text{SbF}_6^-)-$  chains. This model can account for most of the discrepancies between the geometry and vibrational frequencies calculated for the free ions and those observed for solid  $\text{ClF}_4^+\text{SbF}_6^-$ .

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